

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 265 °C

Global applicability domain: Inside

Local applicability domain index: 6.24e-01

Confidence level: 5.72e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Alizarin</div> <div>Measured: 290</div> <div>Predicted: 265</div>	<div>Image not found</div> <div>Rubiadin</div> <div>Measured: 290</div> <div>Predicted: 281</div>	<div>Image not found</div> <div>Danthron</div> <div>Measured: 193</div> <div>Predicted: 207</div>
<div>Image not found</div> <div>1,4-Dihydroxyanthracene-9,10-dione</div> <div>Measured: 200</div> <div>Predicted: 208</div>	<div>Image not found</div> <div>Chrysophanic acid</div> <div>Measured: 196</div> <div>Predicted: 209</div>	